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Internal protein dynamics on ps to μs timescales as studied by multi-frequency 15N solid-state NMR relaxation

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Abstract

A comprehensive analysis of the dynamics of the SH3 domain of chicken alpha-spectrin is presented, based upon 15N T 1 and on- and off-resonance T 1ρ relaxation times obtained on deuterated samples with a partial back-exchange of labile protons under a variety of the experimental conditions, taking explicitly into account the dipolar order parameters calculated from 15N-1H dipole-dipole couplings. It is demonstrated that such a multi-frequency approach enables access to motional correlation times spanning about 6 orders of magnitude. We asses the validity of different motional models based upon orientation autocorrelation functions with a different number of motional components. We find that for many residues a "two components" model is not sufficient for a good description of the data and more complicated fitting models must be considered. We show that slow motions with correlation times on the order of 1-10 μs can be determined reliably in spite of rather low apparent amplitudes (below 1 %), and demonstrate that the distribution of the protein backbone mobility along the time scale axis is pronouncedly non-uniform and non-monotonic: two domains of fast (τ < 10-10 s) and intermediate (10-9 s < τ < 10-7 s) motions are separated by a gap of one order of magnitude in time with almost no motions. For slower motions (τ > 10 -6 s) we observe a sharp ~1 order of magnitude decrease of the apparent motional amplitudes. Such a distribution obviously reflects different nature of backbone motions on different time scales, where the slow end may be attributed to weakly populated "excited states." Surprisingly, our data reveal no clearly evident correlations between secondary structure of the protein and motional parameters. We also could not notice any unambiguous correlations between motions in different time scales along the protein backbone emphasizing the importance of the inter-residue interactions and the cooperative nature of protein dynamics.

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Keywords

Correlation function, Dynamics, Relaxation, SH3 domain, Solid-state